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Why does the rouse model fairly describe the dynamic characteristics of polymer melts at molecular masses below critical mass?

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Abstract

Generalization of the Rouse model without any use of the postulates concerning the Gaussian distribution of the vector connecting the ends of segments is advanced. In the initial (in general, nonlinear) Langevin equations, self-averaging over continuous fragments of a macromolecule naturally defines a linear term for the tagged chain, and this term differs from the entropy term of the classical Rouse model only by the numerical coefficient. According to the inertia-free approximation, the initial decay rates of correlation functions for the normal modes are described by the Rouse model independently of the character of fluctuations of the vector connecting the ends of the Kuhn segment. This statement is valid for any moment if the initial Langevin equations are treated in terms of the approximation of dynamic self-consistency. Simulation of the Fraenkel chains by the method of Brownian dynamics shows that decay of autocorrelation functions of shortwave normal modes is fairly described by the linearized equations for a given model of a chain and that the Rouse equation can be used for the long-wave modes. The results of this study make it possible to explain a marked difference between the lengths of the Kuhn and Rouse segments that is estimated from static and dynamic experiments. © 2010 Pleiades Publishing, Ltd.

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